# Workshop on Emerging Areas of Biological Crystallography

## *Welcome and Opening Remarks*

*Wayne Hendrickson*
*(Columbia University)*

*John Helliwell*
*(University of Manchester)*

*Gopal Shenoy*
*(Advanced Photon Source)*

# Technical Challenges for Biological Crystallography

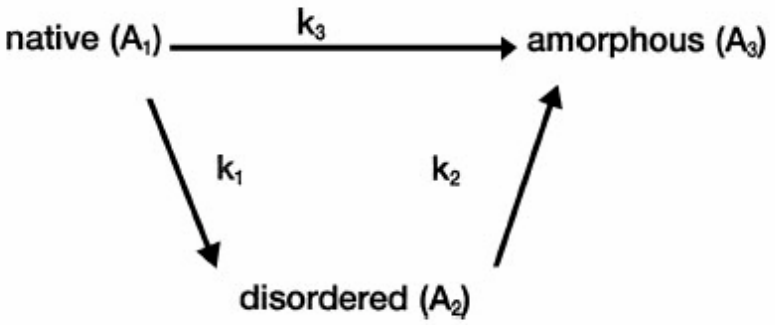
# Technical Challenges - Fundamental

1 Radiation damage

2 Limited crystalline order

# Dose-rate Independent Radiation Damage

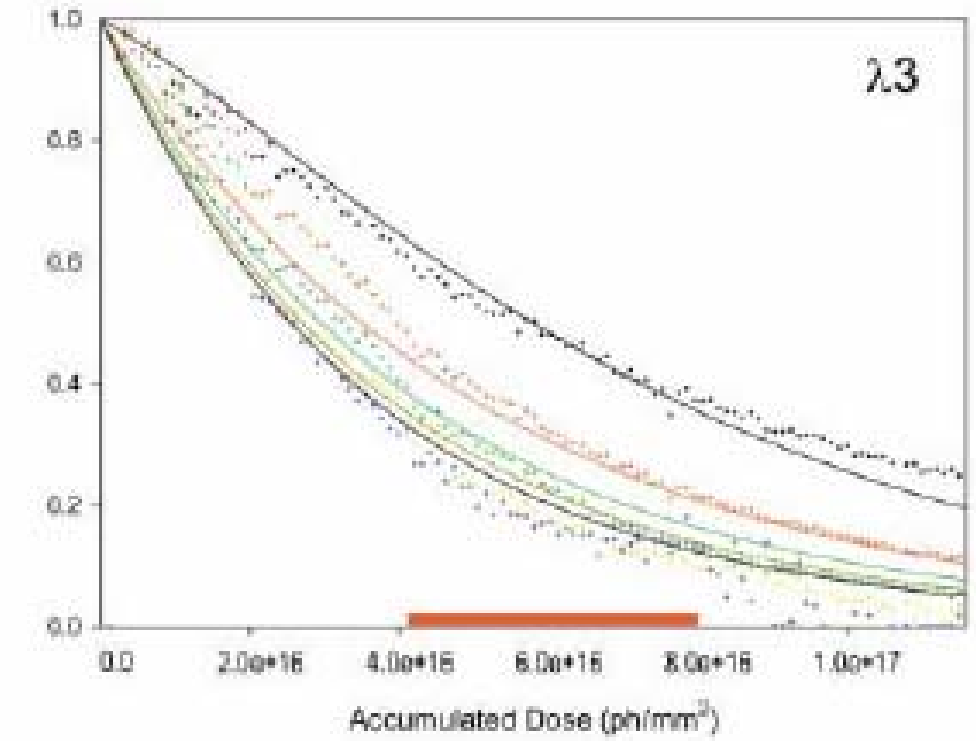
(Sliz, Harrison & Rosenbaum, Structure 11, 13019, 2003)




$$\frac{I(t)}{I_0} = \exp[-(k_1 + k_3)t] + \frac{k_1}{k_1 + k_3 - k_2}\exp(-k_2 t)$$

$$\{1 - \exp[-(k_1 + k_3 - k_2)t]\}\exp\left(-D\frac{\sin^2\theta}{\lambda^2}\right)$$

***$k_3 = 0$***



# Diffraction Intensity and Background

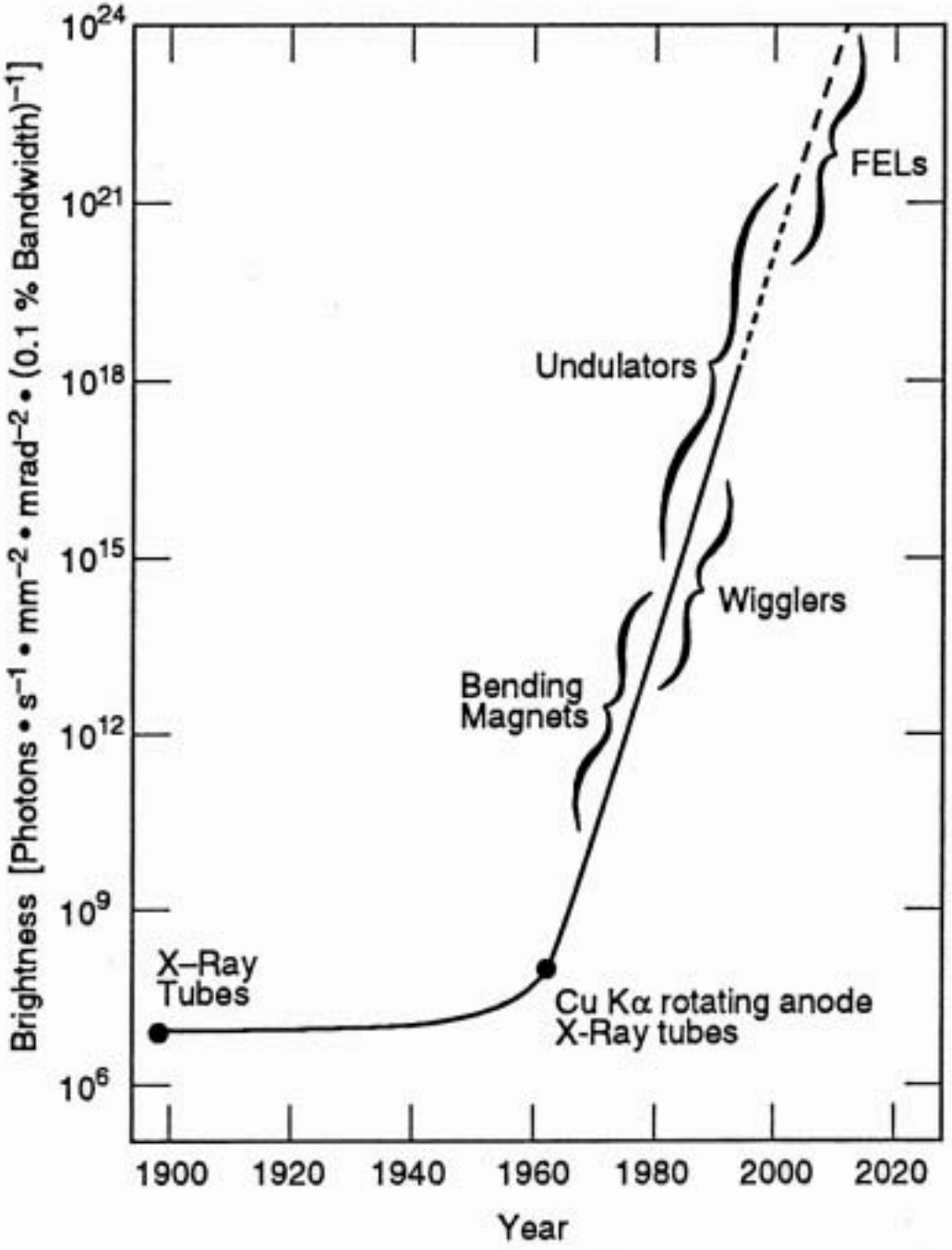
$$\langle I(S) \rangle \propto I_0 \, \omega \, [(1 - S) / V_u] \, \exp(-\tfrac{1}{2} \langle B(S) \rangle S^2) \, V_x$$

$$\langle B(S) \rangle \propto I_0 \, \omega \, \{ [(1 - \exp(-\tfrac{1}{2} \langle B(S) \rangle S^2)] \, V_x + \sigma_p(\lambda) \, V_p + \ldots \}$$

| | | |
|---|---|---|
| $\langle I(S) \rangle$ | $\equiv$ | average Bragg intensity |
| $\langle B(S) \rangle$ | $\equiv$ | average background intensity |
| $I_0$ | $\equiv$ | incident beam intensity |
| $\omega$ | $\equiv$ | rotation speed |
| $S$ | $=$ | $\lvert h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \rvert = 2 \sin(\Theta)/\lambda$ |
| $S$ | $\equiv$ | solvent fraction |
| $V_u$ | $\equiv$ | unit-cell volume |
| $V_x$ | $\equiv$ | illuminated crystal volume |
| $\langle B(S) \rangle$ | $\equiv$ | average atomic mobility factor |
| $\sigma_p(\lambda)$ | $\equiv$ | beampath cross-section |
| $V_p$ | $\equiv$ | beampath volume |

# Technical Challenges - Practical

- Small crystals
- Large unit cells
- Low-resolution structures
- Mega-site sub-structures
- High-throughput


Brightness [Photons • s⁻¹ • mm⁻² • mrad⁻² • (0.1 % Bandwidth)⁻¹]
10²⁴
10²¹
10¹⁸
10¹⁵
10¹²
10⁹
10⁶
1900
1920
1940
1960
1980
2000
2020
Year
FELs
Undulators
Wigglers
Bending Magnets
X-Ray Tubes
Cu Kα rotating anode X-Ray tubes

# Workshop on Emerging Areas of Biological Crystallography

## *Workshop Scope*

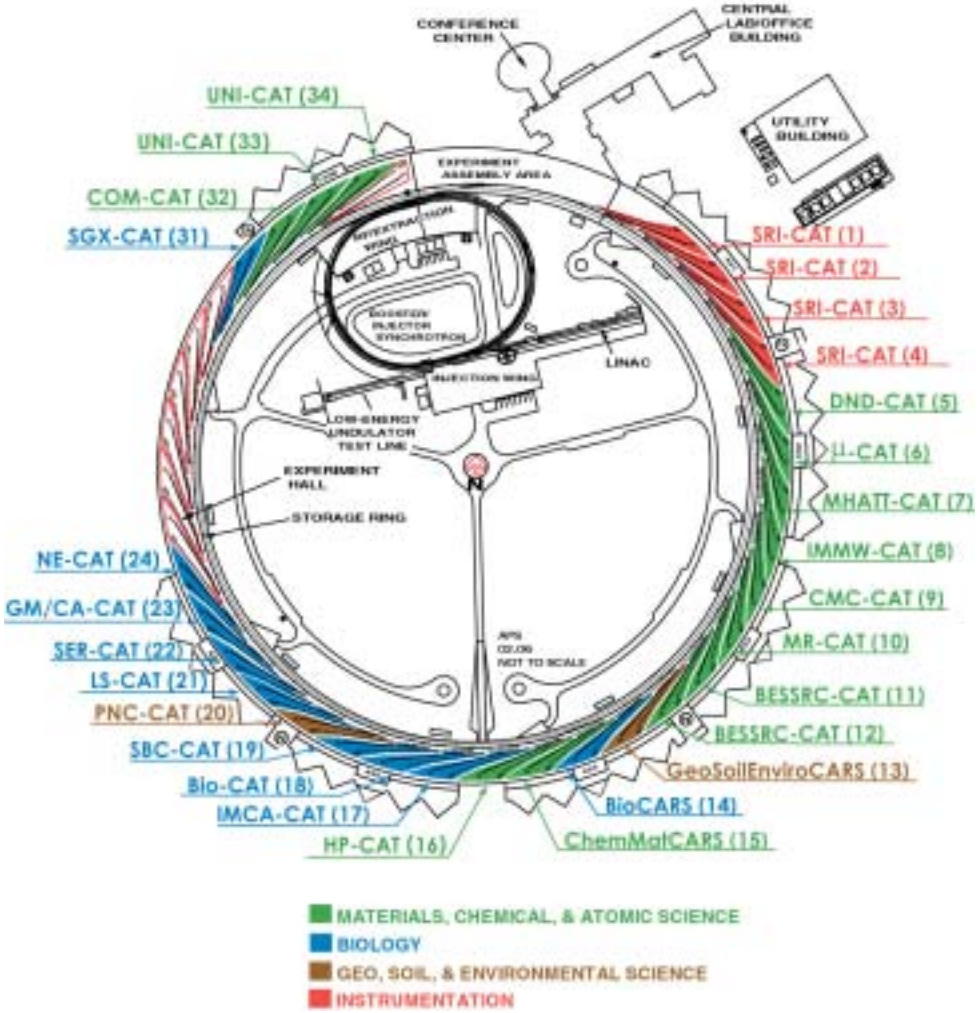
- **Molecular Machines**
- **New Approaches**
- **Radiation Damage**
- **Dynamics**
- **Microfocusing & Coherent Imaging**

# APS Biological Crystallography Capabilities

- BioCARS - Sector 14
- COM - Sector 32
- DND - Sector 5
- GM/CA - Sector 23
- IMCA - Sector 17
- LS - Sector 21
- NE - Sector 24/8
- SBC - Sector 19
- SER - Sector 22
- SGX - Sector 31

# Workshop on Emerging Areas of Biological Crystallography

## *APS Biological Crystallography Capabilities*



# Workshop on Emerging Areas of Biological Crystallography

## *Draft Workshop Objectives*

1. **Explore new and emerging areas defined in the scope of this workshop.**

2. **Broaden the community interaction by including researchers from complementary technologies (e.g. EM, SAXS, NMR, Raman, AFM).**

3. **Identify new scientific proposals/programs specific to the emerging areas in biological crystallography that could be brought to the APS during next 5 to 10 years. Also evaluate the capital and operational requirements for these projects.**

4. **Identify beamline capabilities, beyond those currently available at the APS, that are needed to support research in these emerging areas.**

5. **Address the need and support for theoretical work to strengthen the experimental research.**

6. **Prepare a summary document to serve as a roadmap for the future of the emerging areas in biological crystallography and suggest the role of the Advanced Photon Source towards proposed objectives.**

# Workshop on Emerging Areas of Biological Crystallography

## *Workshop Report*

- **Slides from talks, as provided by the speakers, can be accessed directly by clicking the titles in the program.**
- **You can continually input your thoughts using the 'Swiki' software linked to the lap-top using Wi-Fi**
- **Address the applicable objectives in each of the topics in the scope of the workshop**
- **Input can be made even after the workshop**